

10/576,703

of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 07:59:27 ON 09 MAY 2007

=> file casreact

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'CASREACT' ENTERED AT 07:59:36 ON 09 MAY 2007

USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

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FILE CONTENT:1840 - 5 May 2007 VOL 146 ISS 20

New CAS Information Use Policies, enter HELP USAGETERMS for details.

\*\*\*\*\*  
\* CASREACT now has more than 12 million reactions \*  
\* \*  
\*\*\*\*\*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>  
Uploading C:\Program Files\Stnexp\Queries\10 series\10576703\1.str



chain nodes :

1 2 3 4 5 6 7 8 17 18 19 20 21 22 23 24 27 29 31

ring nodes :

9 10 11 12 13 14 15 16

chain bonds :

Compounds - May 8, 2007

10/576,703

1-2 2-3 2-4 4-5 5-6 6-7 6-8 10-17 12-19 14-18 16-20 21-22 21-27 21-29 23-24  
29-31  
ring bonds :  
9-10 9-13 9-16 10-11 11-12 12-13 13-14 14-15 15-16  
exact/norm bonds :  
9-10 9-13 9-16 10-11 10-17 11-12 12-13 12-19 13-14 14-15 14-18 15-16 16-20  
21-22 21-27 21-29 23-24 29-31  
exact bonds :  
2-4 4-5 5-6  
normalized bonds :  
1-2 2-3 6-7 6-8

G1:H,CH3,CF3,CN,X,[\*1]

G2:C,S,N

G3:Cb,Ak

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:Atom 10:Atom  
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:Atom  
20:Atom 21:Atom 22:CLASS 23:CLASS 24:CLASS 27:CLASS 29:CLASS 31:CLASS  
fragments assigned product role:  
containing 9  
fragments assigned reactant/reagent role:  
containing 1  
containing 21

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 07:59:57 FILE 'CASREACT'

SCREENING COMPLETE - 18 REACTIONS TO VERIFY FROM 2 DOCUMENTS

100.0% DONE 18 VERIFIED 0 HIT RXNS 0 DOCS

SEARCH TIME: 00.00.01

L2 0 SEA SSS FUL L1 ( 0 REACTIONS)

=>

Uploading C:\Program Files\Stnexp\Queries\10 series\10576703\2.str

10/576,703



chain nodes :

9 10 11 12 13 14 15 16 19 21 23

ring nodes :

1 2 3 4 5 6 7 8

chain bonds :

2-9 4-11 6-10 8-12 13-14 13-19 13-21 15-16 21-23

ring bonds :

1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-8

exact/norm bonds :

1-2 1-5 1-8 2-3 2-9 3-4 4-5 4-11 5-6 6-7 6-10 7-8 8-12 13-14 13-19 13-21  
15-16 21-23

G1:H,CH3,CF3,CN,X, [\*1]

G2:C,S,N

G3:Cb,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS

11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 19:CLASS 21:CLASS 23:CLASS

fragments assigned product role:

containing 1

fragments assigned reactant/reagent role:

containing 13

L3 STRUCTURE UPLOADED

=> d

L3 HAS NO ANSWERS

L3 STR

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

Structure attributes must be viewed using STN Express query preparation.

=> s 13 full

FULL SEARCH INITIATED 08:00:21 FILE 'CASREACT'

Compounds - May 8, 2007

10/576,703

SCREENING COMPLETE -        2371 REACTIONS TO VERIFY FROM        244 DOCUMENTS  
100.0% DONE        2371 VERIFIED        5 HIT RXNS        3 DOCS  
SEARCH TIME: 00.00.03

L4                3 SEA SSS FUL L3 (        5 REACTIONS)

=> d ibib hit 1-3